

chain nodes :

8 9 16 18 22 23 24 25

ring nodes :

1 2 3 4 5 6 10 11 12 13 14 15

chain bonds :

5-24 8-11 8-9 8-22 15-16 16-18 22-23 23-24 24-25

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 15-16 16-18 23-24 24-25

exact bonds :

5-24 8-11 8-22 22-23

normalized bonds :

10-11 10-15 11-12 12-13 13-14 14-15

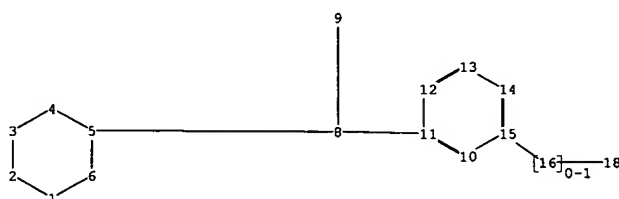
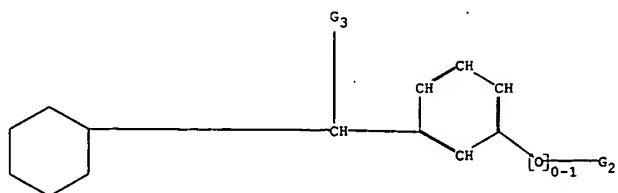
G1:C,O,N

G2:CH3,CF3,Cl,Br,F,CN

G3:CH3,CF3

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 18:CLASS 22:CLASS
23:CLASS 24:CLASS 25:CLASS



chain nodes :

8 9 16 18

ring nodes :

1 2 3 4 5 6 10 11 12 13 14 15

chain bonds :

5-8 8-11 8-9 15-16 16-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 10-11 10-15 11-12 12-13 13-14 14-15

exact/norm bonds :

1-2 1-6 2-3 3-4 4-5 5-6 8-9 15-16 16-18

exact bonds :

5-8 8-11

normalized bonds :

10-11 10-15 11-12 12-13 13-14 14-15

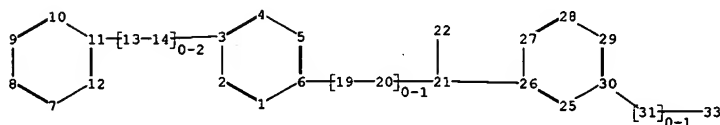
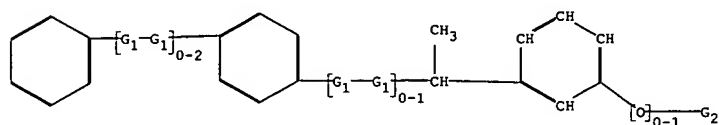
G1:C,O,N

G2:CH3,CF3,Cl,Br,F,CN

G3:CH3,CF3,p-C6H4,CN,Cl,Br,F,I

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:CLASS 10:Atom
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 18:CLASS



chain nodes :

13 14 19 20 21 22 31 33

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 25 26 27 28 29 30

chain bonds :

3-14 6-19 11-13 13-14 19-20 20-21 21-22 21-26 30-31 31-33

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 25-26
25-30 26-27 27-28 28-29 29-30

exact/norm bonds :

3-14 6-19 11-13 13-14 19-20 20-21 30-31 31-33

exact bonds :

21-22 21-26

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 25-26
25-30 26-27 27-28 28-29 29-30

G1:C,O,N

G2:CH3,CF3,Cl,Br,F,CN

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:CLASS 14:CLASS 19:CLASS 20:CLASS 21:CLASS
22:CLASS 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:CLASS
33:CLASS

AN 1992:174144 CAPLUS
 DN 116:174144
 ED Entered STN: 03 May 1992
 TI Preparation of 2-[3-(α -imidazolylbenzyl)phenyl]propanoates and
 analogs as analgesic and antiinflammatory agents
 IN Andreoli Rovati, Romeo; Forne'Felip, Ernesto; Cepero Mestres, Ricardo;
 Carretero Bau, Eduardo
 PA Sociedad Espanola de Especialidades Farmaco-Terapeuticas S. A., Spain
 SO Eur. Pat. Appl., 27 pp.
 CODEN: EPXXDW
 DT Patent
 LA English
 IC ICM C07D233-56
 ICS A61K031-415; C07D233-60; C07D233-61; C07D249-08; C07D295-155;
 C07D409-06; C07D405-06; A61K031-41; A61K031-495; A61K031-38
 CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 1

FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 458160	A2	19911127	EP 1991-107704	19910513
	EP 458160	A3	19920318		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, NL, SE				
	ES 2020463	A6	19910801	ES 1990-1460	19900525
	ES 2029163	A6	19920716	ES 1990-1999	19900725
PRAI	ES 1990-1460	A	19900525		
	ES 1990-1999	A	19900725		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
EP 458160	ICM	C07D233-56
	ICS	A61K031-415; C07D233-60; C07D233-61; C07D249-08; C07D295-155; C07D409-06; C07D405-06; A61K031-41; A61K031-495; A61K031-38

OS MARPAT 116:174144

AB R6OR3 [R3 = H, Ph, alkyl, alkenyl, alkynyl, (CH₂CH₂O)_nH, (CHOH)_mH,
 3-(R₂H)C₆H₄CHR₁X; R₁ = H, Me; R₂ = (un)substituted Ph; R₆ =
 3-(R₂Y)C₆H₄CHR₁X; X = CO, CH₂; Y = CHH, C:CHCH₂A; A = NR₄R₅; R₄, R₅ =
 (phenyl)alkyl; NR₄R₅ = heterocyclyl; n = 1-3; m = 2-4] were prepared as
 analgesics and antiinflammatories (no data). Thus, 3-(PhCO)C₆H₄CHMeCO₂Me
 was reduced and the product treated with SOCl₂ to give
 3-(A₁PhHC)C₆H₄CHMeCO₂Me (I; A = Cl) which was condensed with
 1-(2-thienylmethyl)piperazine to give I [A = 4-(2-
 thienylmethyl)piperazine].

ST imidazolylbenzylphenylpropionate prepn analgesic antiinflammatory

IT Analgesics

Inflammation inhibitors

([(α -imidazolylbenzyl)phenyl]propionates and analogs)

IT	47087-07-0P	55142-64-8P	107257-20-5P	138682-99-2P	138683-00-8P
	138683-01-9P	138683-02-0P	138683-03-1P	138683-04-2P	138683-05-3P
	138683-06-4P	138683-07-5P	139093-60-0P	139093-61-1P	139093-62-2P
	139093-63-3P	139093-64-4P	139093-65-5P	139093-66-6P	139093-67-7P
	139093-68-8P	139093-69-9P	139093-70-2P	139093-71-3P	139093-72-4P
	139093-73-5P	139093-74-6P	139093-75-7P	139093-76-8P	
	139093-77-9P	139093-78-0P	139093-79-1P	139093-80-4P	139093-81-5P
	139093-82-6P	139093-83-7P	139093-84-8P	139093-85-9P	139093-86-0P
	139114-09-3P				

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(preparation and reaction of, in preparation of analgesics and
 antiinflammatories)

IT	138682-91-4P	138682-92-5P	138682-93-6P	138682-95-8P	138682-96-9P
	139093-87-1P	139093-88-2P	139093-89-3P	139093-90-6P	139093-91-7P
	139093-93-9P	139093-94-0P	139093-95-1P	139093-96-2P	139093-97-3P

139093-98-4P 139093-99-5P 139094-00-1P 139094-01-2P 139094-02-3P
 139094-03-4P 139094-04-5P 139094-05-6P 139094-06-7P 139094-07-8P
 139094-08-9P 139094-09-0P 139094-10-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as analgesic and antiinflammatory agent)

IT 39244-79-6 42872-29-7, 3-(1-Cyanoethyl)benzoyl chloride

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, in preparation of analgesics and antiinflammatories)

IT 22071-15-4, 2-(3-Benzoylphenyl)propionic acid

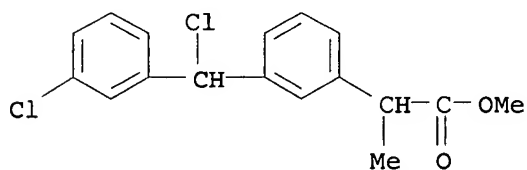
RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, in preparation of analgesics and antiinflammatory agents)

IT 139093-76-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reaction of, in preparation of analgesics and
 antiinflammatories)

RN 139093-76-8 CAPLUS

CN Benzeneacetic acid, 3-[chloro(3-chlorophenyl)methyl]- α -methyl-,
 methyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 1 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2004:993115 CAPLUS
 DN 141:429742
 TI Optically active compounds, their polymers, liquid-crystal compositions,
 and displays
 IN Takeuchi, Kiyofumi; Hasebe, Hiroshi
 PA Dainippon Ink and Chemicals, Inc., Japan
 SO Jpn. Kokai Tokkyo Koho, 24 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	JP 2004323412	A2	20041118	JP 2003-119674	20030424
PRAI	JP 2003-119674		20030424		
OS	MARPAT 141:429742				

L4 ANSWER 2 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2004:100386 CAPLUS
 DN 140:154599
 TI Method of increasing helical twisting power, optically active compound,
 liquid crystal composition containing the same, and liquid crystal display
 device
 IN Nakata, Hidetoshi; Sasaki, Makoto; Takeuchi, Kiyofumi; Takatsu, Haruyoshi
 PA Dainippon Ink and Chemicals, Inc., Japan
 SO U.S. Pat. Appl. Publ., 41 pp.
 CODEN: USXXCO
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004021128	A1	20040205	US 2003-601803	20030624
	JP 2004176038	A2	20040624	JP 2003-154595	20030530
PRAI	JP 2002-189821	A	20020628		
	JP 2002-285617	A	20020930		
OS	MARPAT 140:154599				

L4 ANSWER 3 OF 3 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 2003:646961 CAPLUS
 DN 140:189889
 TI Characteristics of new chiral dopants and their applications
 AU Nakata, Hidetoshi; Sasaki, Makoto; Takeuchi, Kiyofumi; Takatsu, Haruyoshi
 CS Dainippon Ink and Chemicals, Inc., Tokyo, 103-8233, Japan
 SO DIC Technical Review (2003), 9, 29-33
 CODEN: DTREFW; ISSN: 1341-3201
 PB Dainippon Inki Kagaku Kogyo K.K.
 DT Journal
 LA Japanese

AN 2003:646961 CAPLUS
 DN 140:189889
 ED Entered STN: 20 Aug 2003
 TI Characteristics of new chiral dopants and their applications
 AU Nakata, Hidetoshi; Sasaki, Makoto; Takeuchi, Kiyofumi; Takatsu, Haruyoshi
 CS Dainippon Ink and Chemicals, Inc., Tokyo, 103-8233, Japan
 SO DIC Technical Review (2003), 9, 29-33
 CODEN: DTREFW; ISSN: 1341-3201
 PB Dainippon Inki Kagaku Kogyo K.K.
 DT Journal
 LA Japanese
 CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other
 Reprographic Processes)
 Section cross-reference(s): 73, 75
 AB We have investigated properties of new chiral dopants. HTP (Helical
 Twisting Power) of the new dopants are very strong, particularly, a dopant
 which has a substitutional group introduced at meta place in Ph group
 beside chiral center has 25% stronger HTP than dopants without
 substitutional group. Neg. temperature dependence of HTP induced by the chiral
 dopants was observed. The dopant is useful for Cholesteric-LC mixts. to
 improve the operating temperature range and temperature dependence on selective
 reflection wavelength.
 ST chiral dopant helical twisting power cholesteric liq crystal reflection
 IT Phase transition temperature
 (characteristics of new chiral dopants and cholesteric liquid crystals
 with chiral dopants)
 IT Optically active compounds
 RL: MOA (Modifier or additive use); PRP (Properties); USES (Uses)
 (chiral dopants; characteristics of new chiral dopants and cholesteric
 liquid crystals with chiral dopants)
 IT Liquid crystals
 (cholesteric, chiral; characteristics of new chiral dopants and
 cholesteric liquid crystals with chiral dopants)
 IT Electric properties
 (photoelec.; characteristics of new chiral dopants and cholesteric liquid
 crystals with chiral dopants)
 IT Optical reflection
 (temperature dependence of selective reflection wavelength; of new chiral
 dopants and cholesteric liquid crystals with chiral dopants)
 IT 63799-11-1, CB-15 87321-20-8, S-811 156892-43-2 652990-77-7
 652990-79-9 657390-62-0 657390-63-1
 RL: MOA (Modifier or additive use); PRP (Properties); USES (Uses)
 (characteristics of new chiral dopants and cholesteric liquid crystals
 with chiral dopants)
 IT 652990-77-7
 RL: MOA (Modifier or additive use); PRP (Properties); USES (Uses)
 (characteristics of new chiral dopants and cholesteric liquid crystals
 with chiral dopants)
 RN 652990-77-7 CAPLUS
 CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-[(2E)-2-butenyloxy]-,
 (1S)-1-(3-methoxyphenyl)ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry as shown.

